

Exact-exchange density-functional theory for quasi-two-dimensional electron gases

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Abstract

A simple exact-exchange density-functional method for a quasi-two-dimensional electron gas with variable density is presented. An analytical expression for the exact-exchange potential with only one occupied subband is provided, without approximations. When more subbands are occupied the exact-exchange potential is obtained numerically. The theory shows that, in contradiction with LDA, the exact-exchange potential exhibits discontinuities and the system suffers a zero-temperature first-order transition each time a subband is occupied. Results suggesting that the translational symmetry might be spontaneously broken at zero temperature are presented. An extension of the theory to finite temperatures allows to describe a drop in the intersubband spacing in good quantitative agreement with recent experiments.

Density-functional theory (DFT) [1] has been one of the most successful approaches to the problem of interacting particles. The use of the local-density-approximation (LDA) [2] of DFT and related approximations has been widely applied to the study of atoms, molecules, clusters, nuclei, and condensed matter systems. [3,4] At the same time, steady improvements on the experimental techniques have made possible the production of a great number of semiconductor artificial structures that confine the 3D electron gas in one or more dimensions. In particular GaAs/Al_xGa_{1-x}As heterostructures have attracted intense attention, because they are particularly well grown, their conduction band is simple to describe, and they allow the continuous change of the electron density. Because typical 3D electron densities in the quantum well (QW) are very small, the conduction band dispersion can be approximated, without significant error, by a second order expansion around the minimum (effective-mass approximation). [5] As a consequence, the *effective* electron gas formed in the nanostructure can be treated in the frame of Kohn-Sham [2] DFT. All the theoretical techniques developed around DFT and its approximations, such as the LDA, time dependent LDA (TDLDA), spin-density LDA (LSDA) can be tested in these structures which are much easier to modify and control than natural materials [5]. Therefore, semiconductor nanostructures offer the possibility to test over a broad range of conditions the validity of the theoretical tools that are used to describe matter in general.

In this paper we present an approach that goes beyond LDA: an exact-exchange [6,7] density-functional theory for the case of a quasi-two-dimensional electron gas (2DEG). Because we study a metallic system with several subbands occupied, our theory is different than previous exact-exchange (XX) procedures aimed to the study of atoms [6] or bulk semiconductors [7]. Moreover, the number of particles is *not fixed* but it is allowed to fluctuate [3]. When a single subband is occupied we provide an analytical expression for the XX potential *without approximations*. When more subbands are occupied the XX potential is obtained *up to numerical precision*. The implementation of the method is simple enough to replace the state of the art method for 2DEG which is currently based in the LDA. [8] We prove that the XX potential is, in general, a discontinuous function of the density which can

not be accounted by LDA. Therefore, the XX approach yields qualitatively new physics: at zero temperature a first-order transition occurs every time a new subband is occupied. In the transition region, the theory suggest a new phase in which the translational symmetry of the system might be broken. An extension of the theory to finite temperatures allows us to describe a drop in the intersubband spacing when the first-subband is occupied in good quantitative agreement with recent experiments [9].

This theory can be applied to any system with translational symmetry in a plane. For instance, a QW grown epitaxially as shown schematically in Fig. 1a. In these systems, it is possible to confine an electron gas changing the semiconductor in the growth direction z . If the larger gap semiconductor is doped with donors, it provides electrons to the trap formed by the smaller gap semiconductor, until the charge-transfer field equilibrates the chemical potentials in the QW and the doped region (see Fig. 1b). The charge transferred from the doped reservoir to the QW can be tuned by an external electric field [9]. Assuming translational symmetry of the 2DEG in the $x - y$ plane (area A), and proposing accordingly a solution of the type $\phi_{i\mathbf{k}\sigma}(\mathbf{r}) = \exp(i \mathbf{k} \cdot \rho) \xi_i^\sigma(z) / \sqrt{A}$ the ground-state-electron density can be obtained by solving a set of effective one-dimensional Kohn-Sham equations [2] of the form

$$\left[-\frac{1}{2} \frac{\partial^2}{\partial z^2} + V_{KS}(z, \sigma) \right] \xi_i^\sigma(z) = \varepsilon_i^\sigma \xi_i^\sigma(z), \quad (1)$$

where $\hbar^2/(m^* a_0^{*2}) = 2 \text{ Ry}^*$ and a_0^* are the units of energy and length, being m^* the electron effective mass and a_0^* the effective Bohr radius. $\xi_i^\sigma(z)$ is the wave function corresponding to an electron with a spin projection σ (\uparrow or \downarrow), subband index i , and eigenvalue ε_i^σ . In Eq.(1) $V_{KS}(z, \sigma) = V_{ex}(z) + V_H(z) + V_{XX}(z, \sigma) + V_c(z, \sigma)$ is the spin-dependent Kohn-Sham potential given as sum of the external, Hartree, local XX, and correlation potentials, respectively. The external potential is given by the sum of the epitaxial potential plus any external electric field. The zero-temperature 3D electron density $n(z) = \sum_\sigma n(z, \sigma) = \sum_{\varepsilon_i^\sigma < \mu} (\mu - \varepsilon_i^\sigma) |\xi_i^\sigma(z)|^2 / 2\pi$, $n(z, \sigma)$ being the fraction of σ polarized electrons. μ is the chemical potential (or Fermi level) of the system, which is determined by the electrostatic and thermodynamic

equilibrium with a reservoir. $V_H(z)$ is the solution of the Poisson equation. We approximate the *correlation* potential $V_c(z, \sigma)$ as a function of the local spin density [10]. It remains to define the XX potential V_{XX} .

The exchange energy $E_X[n(z, \sigma)]$ of a 2DEG can be obtained through a Slater determinant constructed with the (occupied) self-consistent solutions of Eq. (1), as follows

$$E_X = - \sum_{i,j,\sigma} k_F^{i\sigma} k_F^{j\sigma} \int dz dz' \varphi_i^\sigma(z, z') \varphi_j^\sigma(z', z) F_{ij}^{11}(z, z'), \quad (2)$$

where $\varphi_i^\sigma(z, z') = \xi_i^\sigma(z)^* \xi_i^\sigma(z')$, $F_{ij}^{mn}(z, z') = \frac{A}{4\pi} \int \frac{d\rho}{\rho^{m+n-1}} \frac{J_m(k_F^{i\sigma} \rho) J_n(k_F^{j\sigma} \rho)}{\sqrt{\rho^2 + (z - z')^2}}$, $k_F^{i\sigma} = \sqrt{2\theta(\mu - \varepsilon_i^\sigma)} (\mu - \varepsilon_i^\sigma)^{1/2}$, $\theta(x)$ is the step function, and $J_n(x)$ stands for the cylinder Bessel function of order n . The XX potential $V_{XX}(z, \sigma)$ can be obtained from

$$V_{XX}(z, \sigma) = \frac{\delta E_X}{\delta n(z, \sigma)} = A \sum_i \int dz' \frac{\delta V_{KS}(z', \sigma)}{\delta n(z, \sigma)} \times \left\{ \int dz'' \left[\frac{\delta E_X}{\delta \xi_i^\sigma(z'')} \frac{\delta \xi_i^\sigma(z'')}{\delta V_{KS}(z', \sigma)} + c.c. \right] + \frac{\delta E_X}{\delta k_F^{i\sigma}} \frac{\delta k_F^{i\sigma}}{\delta V_{KS}(z', \sigma)} \right\}. \quad (3)$$

The first term in the r.h.s. of Eq.(3) comes from functional derivatives with respect to the “shape” of the wave function [7], while the second term is a result of changes in the occupation of the subbands and has not been considered in previous XX treatments for fixed particle-number systems. $\delta V_{KS}(z', \sigma) / \delta n(z, \sigma) \equiv \chi_\sigma^{-1}(z, z')$ is the inverse of the operator $\chi_\sigma(z, z') \equiv \delta n(z, \sigma) / \delta V_{KS}(z')$ given by

$$\chi_\sigma(z, z') = \sum_i \left\{ \frac{(k_F^{i\sigma})^2}{4\pi A} [\varphi_i^\sigma(z, z') G_{i\sigma}(z, z') + c.c.] - \frac{f(\varepsilon_i^\sigma)}{2\pi A} |\varphi_i^\sigma(z, z')|^2 \right\}, \quad (4)$$

being $G_{i\sigma}(z, z') = \sum_{j(\neq i)} \varphi_j^\sigma(z', z) / (\varepsilon_i^\sigma - \varepsilon_j^\sigma)$, and $f(\varepsilon_i^\sigma) = 1 / [1 + \exp((\varepsilon_i^\sigma - \mu) / k_B T)]$ the Fermi occupation factor [11]. The first term in Eq.(4) comes from first-order perturbation theory [12], whereas the second term results from first-order perturbation theory and the thermodynamic equilibrium between the 2DEG and the reservoir that fixes a common chemical potential μ allowing the change of the number of particles. Indeed, without this second term, the operator $\chi_\sigma(z, z')$ in general cannot be inverted because it is singular [6,7]. Eq.(3)

could be brought to an alternative expression, which allows the discussion of our approach in the context of the Optimized Potential Method (OPM). [13] For this, we multiply Eq.(3) by $\chi_\sigma(z, z')$, and integrate over all z . Proceeding this way, it could be rewritten as

$$\sum_i (k_F^{i\sigma})^2 \int dz' \{ [V_{XX}(z', \sigma) - v_{X,i}(z', \sigma)] G_{i\sigma}(z', z) \varphi_i^\sigma(z', z) + c.c. \} - 2 \sum_i^{occ} |\xi_i^\sigma(z)|^2 \left[\bar{V}_{XX,i}(\sigma) - \frac{2\pi}{A k_F^{i\sigma}} \frac{\delta E_X}{\delta k_F^{i\sigma}} \right] = 0. \quad (5)$$

Here, $v_{X,i}(z, \sigma) = [4\pi/A(k_F^{i\sigma})^2 \xi_i^\sigma(z)^*] \delta E_X / \delta \xi_i^\sigma(z)$, and $\bar{V}_{XX,i}(\sigma)$ is the diagonal matrix element of $V_{XX}(z, \sigma)$ with $\xi_i^\sigma(z)$. This integral equation for $V_{XX}(z, \sigma)$ is the generalization of the OPM to our open configuration, where the system is free to exchange particles with the surroundings; for a closed system (fixed number of particles), the last term on the r.h.s. of Eq.(5) is zero, and the integral equation reduces to the one of the standard OPM for atoms and molecules. [13] Some consequences of Eq.(5) are worth of address: *a)* the solution for $V_{XX}(z, \sigma)$ is *univocally* determined, including the (possible) presence of a constant shift C ; *b)* its solution in the one-subband case $i = 0$ is immediate: Replacing $V_{XX}^0(z, \sigma) = v_{X,0}(z, \sigma) + C$ in Eq.(5) and solving for C , we found

$$V_{XX}^0(z, \sigma) = -\frac{8\pi}{A} \left\{ \int dz_1 \varphi_0^\sigma(z_1, z_1) F_{00}^{11}(z_1, z) + k_F^{0\sigma} \int dz_1 dz_2 |\varphi_0^\sigma(z_1, z_2)|^2 \left[\frac{F_{00}^{01}(z_1, z_2)}{2} - \frac{F_{00}^{11}(z_1, z_2)}{k_F^{0\sigma}} \right] \right\}. \quad (6)$$

Using Eq.(6) it can be shown that $\int V_{XX}^0(z, \sigma) [\xi_0^\sigma(z)]^2 = dE_X/dN_\sigma = \mu_X^\sigma$, with E_X given by Eq.(2), $N_\sigma = \int d\mathbf{r} n(z, \sigma)$ the total number of electrons with spin σ , and μ_X^σ the exchange contribution to the total chemical potential μ . Accordingly, the Janak theorem [14] is explicitly satisfied in our XX-DFT formalism. Besides, when Eq.(6) is particularized to the strict 2D limit by imposing the condition $[\xi_0^\sigma(z)]^2 \rightarrow \delta(z)$ [$\delta(z)$ being the Dirac delta function], we obtain $V_{XX}^0(0, \sigma) = -2k_F^{0\sigma}/\pi$, which is exactly the well known value of the exchange contribution to the chemical potential for an homogeneous 2D electron gas. In other words, Eq.(6) contains the exact 2D limit of the exchange potential. [15] Finally *c)*, for two (or more) occupied subbands, the analytical exact solution of our OPM integral equation is unknown. Some progress can be achieved following the Sharp-Horton (SH) or KLI approximation [13] of the

orbital Green function $G_{i\sigma}(z, z')$. It amounts to replace the denominators $(\varepsilon_i^\sigma - \varepsilon_j^\sigma)$ by an orbital independent average $\Delta\tilde{\varepsilon}_\sigma$; substituting $G_{i\sigma}(z, z') \simeq [\delta(z - z') - \sum_i |\varphi_i^\sigma(z, z')|^2] / \Delta\tilde{\varepsilon}_\sigma$ in Eq.(5) one obtains an explicit solution for $V_{XX}(z, \sigma)$, which will be given elsewhere. [16] For the one-subband case, the KLI approximation leads to the exact result, given by Eq.(6). But for the multi-subband case ($i \geq 1$), and because of the second term in Eq.(5), the explicit solution for $V_{XX}(z, \sigma)$ becomes $\Delta\tilde{\varepsilon}_\sigma$ dependent, in contrast with the situation for atoms and molecules. [13]

As proceeding along this line of work would had forced us to introduce a new and unknown scale of energy ($\Delta\tilde{\varepsilon}_\sigma$), we studied the multi-subband case by directly solving Eq.(4). The fundamental ingredient for this direct approach is an analytical limit for $\chi_\sigma^{-1}(z, z')$. For $T = 0$ and in the case where *only* the ground state subband is occupied $\chi_{0\sigma}^{-1}(z, z') = \sum_i d_i^\sigma \psi_i^\sigma(z) \psi_i^\sigma(z')$, where $d_0^\sigma = -2$, $d_{i>0}^\sigma = -(\varepsilon_i^\sigma - \varepsilon_0^\sigma) / (\mu - \varepsilon_0^\sigma)$, and $\psi_i^\sigma(z) = \xi_i^\sigma(z) / \xi_0^\sigma(z)$. Replacing this and Eq.(2) into (3) we get again, by a different method, Eq.(6). For many occupied subbands, one can obtain $V_{XX}(z, \sigma)$ using Eq.(3) because $\chi_\sigma^{-1}(z, z')$ can be obtained recursively in terms of $\chi_{0\sigma}^{-1}(z, z')$ for any number of bands and temperature, by using the Sherman-Morrison method. [17] Thus for more than one subband we have evaluated $V_{XX}(z, \sigma)$ up to numerical precision. In order to test the numerical method we verified that, in double quantum well systems with *two* occupied subbands, the *single* subband analytical limit for the XX potential in one well (Eq.(6)), is nicely reproduced numerically as we increase the barrier between the wells.

Fig.1b gives the full self-consistent potential $V_{KS}(z)$ and the squared wave functions $[\xi_i^\sigma(z)]^2$ corresponding to the first four states. The results were obtained for a QW of GaAs in $\text{Al}_x\text{Ga}_{1-x}\text{As}$ with a band offset of 220 meV and a width of 245 Å. The structure is doped on one side at 135 Å from the left QW edge with a 3D dopant density of $2 \times 10^{18}/\text{cm}^{-3}$. Without external electric field and at zero temperature the ground state is paramagnetic, the intersubband spacings are $E_{01} = \varepsilon_1^\sigma - \varepsilon_0^\sigma = 26.78$ meV, $E_{02} = 60.58$ meV, $E_{03} = 108.36$ meV, while $\mu - \varepsilon_0^\sigma = 24.14$ meV is just below $\varepsilon_1^\sigma - \varepsilon_0^\sigma$ and only one subband is occupied.

In Fig.2 we compare the potential $V_{XX}^0(z, \sigma)$ corresponding to Fig.1b [obtained using

Eq.(6)] with the exchange potential in LDA $V_x^{LDA}(z, \sigma) = -[6n(z, \sigma)/\pi]^{1/3}$ for the *same* XX density. Note that although V_x^{LDA} and V_{XX}^0 have a similar amplitude in the QW region, their respective asymptotic behaviors are completely different: while V_x^{LDA} goes exponentially to zero for $|z| \rightarrow \infty$, V_{XX}^0 tends asymptotically (as $-1/|z|$) towards the constant (positive) contribution of Eq.(6). This results in larger intersubband spacings using XX theory for the same total electron density. Note that the minimum of $V_{XX}^0(z, \sigma)$ is not at the maximum of $n(z, \sigma)$ as in $V_x^{LDA}(z, \sigma)$ and also note that $V_{XX}^0(z, \sigma)$ is large where $n(z, \sigma)$ is negligible. Both features are consequences of the non-local dependence of $V_{XX}^0(z, \sigma)$ on $n(z, \sigma)$, displayed explicitly in Eq.(6).

Significant qualitative differences between LDA and XX theory appear each time a new subband is occupied. For instance in Eq.(3), at zero temperature, a finite term proportional to $\delta E_X/\delta k_F^{1\sigma}$ appears discontinuously [9] when $k_F^{1\sigma} \rightarrow 0^+$. Moreover, in Eqs.(4) and (5), when $\mu \rightarrow \varepsilon_1^\sigma + 0^+$, a finite contribution $(-|\varphi_1^\sigma(z, z')|^2/2\pi A)$ appears in the second term. Therefore, the inverse $\chi_\sigma^{-1}(z, z')$ also changes discontinuously when $k_F^{1\sigma} \rightarrow 0^+$. Although the discontinuities in $\delta E_X/\delta k_F^{1\sigma}$ and χ_σ^{-1} have opposite effects, they do not cancel each other and χ_σ^{-1} dominates [16]. Let us consider what happens when μ crosses a subband energy ε_n^σ but one neglects the self-consistent adjustments of the charge. In that case, because of the discontinuities introduced by $\delta E_X/\delta k_F^{1\sigma}$ and in χ_σ^{-1} , the XX potential must change discontinuously:

$$V_{XX}(z, \sigma, \mu \rightarrow \varepsilon_n^\sigma + 0^+) = V_{XX}(z, \sigma, \mu \rightarrow \varepsilon_n^\sigma - 0^+) + \Delta V_{XX}^{n-1, n}(z, \sigma). \quad (7)$$

Therefore, the wave functions, the total electron density, and the total energy cannot be continuous functions of μ and the discontinuity $\Delta V_{XX}^{n-1, n}$ signals a first-order transition of the 2DEG. An interesting question is what is the effect of $\Delta V_{XX}^{0, 1}(z, \sigma)$ on the intersubband spacing E_{01} . Case I: if one only considers the discontinuities in $\delta E_X/\delta k_F^{1\sigma}$, $E_{01}(\mu \rightarrow \varepsilon_1^\sigma + 0^+) < E_{01}(\mu \rightarrow \varepsilon_1^\sigma - 0^+)$ and μ lies above the first-excited subband and a *finite* amount of charge is abruptly transferred from the ground to the first-excited subband. Case II: if one adds the discontinuities in χ_σ^{-1} , $E_{01}(\mu \rightarrow \varepsilon_1^\sigma + 0^+) > E_{01}(\mu \rightarrow \varepsilon_1^\sigma - 0^+)$ and μ remains below

the bottom of the first-excited subband and a self-consistent solution of the system is not possible (under our assumption of translational symmetry). In words, if the system attempts the occupation of the first-excited subband, this increases the intersubband spacing, which in turn empties the excited subband in the next iteration, which in turn produces a lower intersubband spacing, and so on. Finally, if $E_{01}(\mu \rightarrow \varepsilon_1^\sigma + 0^+) = E_{01}(\mu \rightarrow \varepsilon_1^\sigma - 0^+)$ (Case III) a smooth occupation of the first-excited subband would be possible. Provided that self-consistency is frozen, the only possibility in the LDA is Case III, because the LDA exchange potential is a continuous function of the density. Self-consistent effects, in some conditions, can generate first-order transitions within LDA [8]. But in XX theory, in contrast, a second order transition will be an accident and, in general, first-order transitions are expected when μ crosses a subband energy at zero temperature. [18]

In Fig.3 we plot the intersubband spacing E_{01} as a function of the total 2D electron density $N/A = (N_\uparrow + N_\downarrow)/A$ with different methods. The dotted line corresponds to the usual LDA, the continuous line to XX theory at zero temperature, and the dashed line was obtained with an approximated [11] finite temperature XX theory ($T = 10$ K in Eq.(4)). The straight line is the evolution of $\mu - \varepsilon_0^\sigma = (\pi\hbar^2/m^*)N/A$ in an hypothetical system with a single band occupied. All methods give similar qualitative results when E_{01} is far from $\mu - \varepsilon_0^\sigma$, though LDA calculations give smaller intersubband spacings than XX methods (as expected from Fig.2). However, significant qualitative differences appear when $E_{01} \approx \mu - \varepsilon_0^\sigma$. The LDA calculation gives a continuous curve but there is a discontinuity in the derivative of E_{01} when the first-excited subband is occupied (which implies a second order transition). The zero temperature calculations with XX theory give a remarkable result: there is a window of densities where a self-consistent solution is not achieved because it corresponds to the Case II discussed above. Our interpretation of this window, where it is not possible to find a self-consistent solution under the assumption of translational invariance, is that this symmetry must be broken in the ground state. Thus in this density region a new broken symmetry phase might exist at low temperatures.

Consideration of finite temperatures in Eq.(4) introduces smoothly the discontinuity in

$\chi_{\sigma}^{-1}(z, z')$ when $|\mu - \varepsilon_1^{\sigma}| \approx k_B T$. This allows us to achieve a self-consistent solution for all densities (although the numerical convergence becomes unstable in some cases). As the density increases, the occupation of the first-excited subband cannot be avoided and $\delta E_X / \delta k_F^{1\sigma}$ generates a sudden drop in E_{01} . This new solution is also stable at lower densities. Accordingly, there is a range of densities where it is possible to find *two* solutions. A first-order transition occurs when the free energies of the two solutions cross; detailed temperature-dependent calculations will be reported elsewhere. From Fig.3 we can estimate the drop on E_{01} considering the energies in the density range where the two solutions exist: $\Delta E_{01} = 2.4 \pm 0.4$ meV, which is in very good agreement with the measurement of 3.5 meV reported by Goñi *et al.* [9].

In summary we have extended the KS-DFT for 2DEG beyond the state of the art method based on the LDA. Our theory allows to obtain an exact exchange potential without approximations up to numerical precision, while correlations are considered in the LDA level. The theory satisfies known limits and theorems. The theory predicts first-order transitions every time a new subband is occupied and suggest that for some systems at zero temperature the translational symmetry might be spontaneously broken. Finite temperature effects are included approximately. We calculated the self-consistent solutions for a realistic system and obtained phase transitions which are in good quantitative agreement with recent experiments.

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FIGURES

FIG. 1. (a) Schematic representation of an asymmetric doped quantum well nanostructure. (b) Self-consistent subband structure and self-consistent potential for the zero-bias situation.

FIG. 2. Comparison of the exact exchange potential with the LDA potential when only one subband is occupied. The full upper line is the 3D density $n(z)$ obtained with XX theory (corresponding to a 2D density of $0.68 \times 10^{12}/\text{cm}^2$). XX and LDA exchange potentials are compared for this same density. Energies are measured from the chemical potential μ .

FIG. 3. Intersubband spacing E_{01} as a function of the 2D density N/A . Full lines, zero temperature exact exchange; dashed lines, finite temperature exact exchange; dotted line, LDA.